Proposals Funded from those received under Office of Science Solicitation 3-16 and DOE Laboratory Announcement 3-16
Catalysis Science

Three-year proposed funding amounts are contingent on the availability of Congressionally-appropriated funds.

1. University of Delaware - $1,773,000

Title: "From First Principles Design to Realization of Bimetallic Catalysts for Enhanced Selectivity"

PIs: U. of Delaware: Mark Barteau, D. Buttrey, J. Chen, J. Lauterbach, R. Lobo and D. Vlachos. TAMU: R. Crooks. U. Wisconsin: M. Mavrikakis, J. Dumesic.

Scope: The objective of the work is to demonstrate a comprehensive theoretical-experimental approach to the design of selective catalytic functions. Bimetallic surfaces and particles will provide the versatile platform whose atomic constitution will be tailored and preserved to guide specific reactants towards specific products. The disciplinary components include theory and modeling; surface science; materials synthesis; characterization and scale-up; and catalyst and reactor dynamics and optimization. The target reactions will be the selective hydrogenation of multifunctional hydrocarbons, chemoselective oxidation of olefins, and selective reforming of carbohydrates to alkanes.

2. Cleveland State University - $1,095,000

Title: "Electron Transport, Oxygen Activation and Biosynthesis: An Integrative Electrochemical and Computational Approach"

PIs: Mekki Bayachou, V. Gogonea, A. Zhou

Scope: This work entails the biochemical, electrochemical, quantum mechanical and molecular dynamics study of elementary processes in the biosynthesis of NO catalyzed by P450-NOS. In particular, it focuses on acquiring mechanistic understanding of the electron transport, the oxygen activation and the catalytic cycle for NO synthesis.

3. Purdue University - $2,240,257

Title: "Catalyst Design by Discovery Informatics"

PIs: W. Nicholas Delgass, J. Caruthers, R.G. Crooks, H. Hillhouse, F. Ribeiro, I. Rothwell, K. Thomson, V. Venkatasubramaniam

Scope: The objective of the work is to develop new methodology for catalysis research, involving theory, experimentation, and information science to identify quantitative relationships between the chemical structure and composition of catalysts and reactants, and the catalytic behavior.

4. Columbia University - $1,710,000

Title: "Controlling Structural, Electronic, and Energy Flow Dynamics of Catalytic Processes through Tailored Nanostructures"

PIs: Columbia: Tony Heinz, S. O'Brien; UCRiverside: L. Bartels; Kansas St. U.: T. Rahman

Scope: The goal of this work is to develop a fresh approach to uncover what determines selectivity in catalysts and to construct new catalysts using such knowledge. In particular, this team proposes to exploit the steric and entropic control over the diffusion motion and reaction energy, respectively. The work will involve collaboration among experts in the analysis of surface reactions on the atomic time and length scale with experts in synthetic methods appropriate for nanoscale structures.

5. Georgia Tech Research Corporation - $1,866,000

Title: "Basic Principles that Govern the Interaction of Organometallic Catalysts with Supports – the Science of Immobilized Molecular Catalysts"

PIs: Christopher W. Jones, M. Weck, P.J. Ludovice, C.D. Sherrill; U. Va.: R.J. Davis

Scope**:** This work will unveil fundamental aspects of immobilized organometallic catalysts through a combination of synthesis, characterization, catalysis and molecular modeling/electronic structure studies focused on the dynamic properties of the organometallic-ceramic interfaces. The proposal addresses to a large extent the stated goal of bridging the gap between homogeneous and heterogeneous catalysis by endowing solid substrates with designed molecular functionalities.

6. Emory University - $903,945

Title: "Principles of Selective O_2-Based Oxidation by Optimal (Binuclear) Catalytic Sites"

PIs: Djamaladdin Musaev, Craig Hill, Keiji Morokuma

Scope: The goal of this work is to establish the fundamental principles that control the reactivity of substituted polyoxometalates (POMs) in the oxidation of organic substrates by O_2. The research will result in new theoretical-experimental methodology to treat supramolecular inorganic catalysts and predict their reactivity and stability.

7. University of California – Santa Barbara - $1,342,000

Title: "Hierarchical Design of Heterogeneous Catalysis for Hydrocarbon Transformations: Structures and Dynamics of the Active Sites"

PIs: Susannah Scott, B. Chmelka, J. Eckert

Scope: The objective of the work is to develop fundamental understanding of how the environment provided by a hierarchical inorganic structure controls the reactivity and stability of the organometallic transition metal complexes grafted in the hybrid materials as catalytic functionalities. Experts in materials synthesis, organometallic chemistry, structural analysis by x-ray absorption and NMR, labile intermediate characterization by inelastic neutron scattering and NMR, and molecular modeling, are brought to bear on the multiple complexities of this important topic.

8. University of Pittsburgh – $892,612

Title: "The Reactivity and Structural Dynamics of Supported Metal Nanoclusters Using Electron Microscopy, In Situ X-Ray Spectroscopy, Electronic Structure Theories, and Molecular Dynamics Simulations"

PIs: Judith Yang; U. Illinois: D. Johnson, R. Nuzzo ; Yeshiva U. : Frenkel

Scope: The objective of the work is to develop detailed information and fundamental understanding of the atomic restructuring and time-dependent behavior of catalytic metal nanoparticles in the form of ligand-bound clusters or denuded clusters stabilized on inorganic supports or embedded in organic matrices. The work will involve a collaborative team to carry out synthesis, high-resolution imaging, synchrotron x-ray absorption spectroscopies, first-principles theory, and computational modeling.

9. University of California – Riverside - $1,685,000

Title: "Molecular-Level Design of Heterogeneous Chiral Catalysts"

PIs: UCRiverside: Francisco Zaera; Carnegie-Mellon U.: D. Sholl, A. Gellman ; U. Wisc.-Milw. : E. Tysoe

Scope: The objective of the work is to identify the fundamental mechanisms that cause chiral selectivity in heterogeneous catalysis. An integrated experimental and theoretical approach will be implemented to understand the complex behavior of catalytic surfaces that exert chiral resolution upon reacting prochiral substrates.

10. Pacific Northwest National Laboratory - $4,790,505

Title: "Early Transition Metal Oxides as Catalysts: Crossing Scales from Clusters to Single Crystals to Functioning Materials"

PIs: PNNL: David A. Dixon, D. Peden, B. Kay, J.Z. Hu, A. Dohnalek, M. Gutowski, and Y. Wang; UCBerkeley: E. Iglesia; SNL: J. Liu; U. Texas: J.M. White; Washington St. U.: L.S. Wang

Scope: The objective of the project is to develop an integrated experimental-theoretical approach to the molecular-level study, design, and control of transition-metal oxide catalysts, specifically for redox and acid-base chemical reactions. From the simpler to the more complex chemistry, the model reactions are: dehydration of butanol, selective oxidation of methanol, selective oxidation of alkanes, and isomerization-alkylation of alkanes. The approach combines solid-state inorganic synthesis, surface science, experimental and theoretical-computational chemical physics, and mechanistic organic chemistry to address the challenge.

11. Ames National Laboratory - $1,835,000

Title: "Selective and Efficient Catalysis in 3-D Controlled Environments"

PIs: Marek Pruski, V. Lin, A. Bakac, J. Espenson, R. Angelici

Scope: The goal of the work is to understand how to coalesce the best features of homogeneous and heterogeneous catalysts into single 3-D domains. Namely, this project will lead to the synthesis of complex mesoporous architectures with controlled morphology, external surface chemistry, functionalized pore entrances, and internal spatial distribution of multiple chemical functions. The new designs will possess tunable activity, selectivity and deactivation characteristics for several classes of reactions, including enantioselective hydrogenation, hydrolysis, polymerization and oxidation of complex multifunctional organic molecules. Structural and mechanistic aspects key to catalytic performance will be determined by a combination of physical and chemical methods, including also theory and simulation.